Contribution to the theory of inelastic neutron scattering in superfluid helium

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The Keldysh diagram technique is used to investigate the line shape of roton creation by a slow neutron in superfluid helium. It is shown that this shape is determined by the same roton-roton scattering probability as the kinetic coefficients of helium in the roton region. The line shape differs from Lorentzian in that the intensity falls off more rapidly on the negative wing.

1. INTRODUCTION

The aim of the present paper is a microscopic calculation of the probability of roton production in scattering of low neutrons in superfluid helium with allowance for the interaction between the rotons.

Slow-neutron scattering is known to be an important tool in the investigation of liquid helium. Recent improvements of the experimental technique permit a substantial increase of the resolution and make possible a detailed investigation of the roton line shape.[1] A theoretical calculation of this shape is therefore most vital. We shall see that this shape has singularities connected with a specific roton-dispersion law.

The first to investigate the roton line shape was apparently Cohen.[2] Using the diagram technique of Bloch and de Dominicis, he expressed the roton-creation dynamic form factor in terms of a roton-roton scattering matrix. He did not investigate, however, the line shape in sufficient detail. This is why it is usually stated in later papers that Ref. 2 leads only to a pure Lorentz line shape, a statement we shall show below not to be valid in the entire energy-transfer region.

The next step towards the solution of the problem was made by Halley and Hastings.[3,4] They expressed the scattering probability in terms of the imaginary part of the roton retarded Green's function, thereby facilitating the calculations. Even they, however, did not engage in an actual calculation of this function. In addition, they used in the transformations the symmetry relation for the self-energy functions, a relation not vlaid in the general case (see footnote 2 below).

2. ROTON CREATION PROBABILITY IN THE KELDYSH DIAGRAM TECHNIQUE

It is known that the neutron scattering probability is expressed in terms of the dynamic form factor of the liquid $S(\varepsilon,\mathbf{p})$, which is the Fourier component of the expectation value with respect to space and time

$$S(\varepsilon,\mathbf{p})=\frac{1}{\bar{n}}\langle\delta n(t,\mathbf{r})\,\delta n(0,0)\rangle_{\varepsilon,\mathbf{p}},\tag{1}$$

where δn stands for the fluctuations of the atom-number density of the liquid, and $\bar{n}$ is the average density of the atoms. Just as in Refs. 2–4, we shall assume that roton creation and absorption are described by a term that is linear in the roton creation and annihilation operators and has the form

$$\delta n=[\bar{n}\xi(\mathbf{p})]^{1/2}(\hat{a}_{\mathbf{p}}^{+}+\hat{a}_{-\mathbf{p}})\tag{2}$$

with a certain coefficient $\xi(\mathbf{p})$.

We are interested in the present paper only in the line broadening (and not in its shift). Since processes with change of the number of rotons are known to have low probability[1)] (Ref. 5), we shall, in contrast to Ref. 3, disregard them. In other words we assume, as in Ref. 2, that the interaction Hamiltonian conserves the number of rotons. It follows then from Eqs. (1) and (2) that

$$S(\varepsilon,\mathbf{p})=\xi(\mathbf{p})\,[iG^{+-}(\varepsilon,\mathbf{p})+iG^{-+}(-\varepsilon,\mathbf{p})],\tag{3}$$

where $G^{+-}(\varepsilon,\mathbf{p})$ and $G^{-+}(\varepsilon,\mathbf{p})$ are respectively the Fourier components of the functions

$$\begin{aligned}iG^{+-}(\mathbf{r},t)&=\langle\Psi(\mathbf{r},t)\Psi^{+}(0,0)\rangle,\\ iG^{-+}(\mathbf{r},t)&=\langle\Psi^{+}(0,0)\Psi(\mathbf{r},t)\rangle\end{aligned}\tag{4}$$

(we use a system of units in which $\hbar=1$). Here $\Psi^{+}(\mathbf{r},t)$ and $\Psi(\mathbf{r},t)$ are the roton creation and annihilation operators in the **r**-representation and are connected with $\hat{a}^{+}$ and $\hat{a}$ in the usual manner, while the functions G^{+-} and G^{-+} are two of the four functions involved in the Keldysh diagram technique (see Ref. 6; we use the notation of Ref. 7). Equation (3) makes therefore possible a consistent calculation of the form factor $S(\varepsilon,\mathbf{p})$. The first term of this equation describes roton creation, and the second absorption. To be specific, we shall be interested only in creation, i.e., consider only the first term.

Besides the function G^{+-} and G^{-+} we shall need also the usual Feynman Green's function, which we denote in this connection by G^{--}, and also the function G^{++}, where

$$G^{++}(\varepsilon,\mathbf{p})=-[G^{--}(\varepsilon,\mathbf{p})]^{*}.\tag{5}$$

Expressing $G^{+-}(\varepsilon,\mathbf{p}),G^{-+}(\varepsilon,\mathbf{p})$ and $G^{--}(\varepsilon,\mathbf{p})$ in the usual manner in terms of the matrix elements of the Ψ operators, we readily show that in the thermodynamic equilibrium state

$$\begin{aligned}G^{+-}(\varepsilon,\mathbf{p})&=i\,[1+\mathrm{th}(\varepsilon/2T)]\,\mathrm{Im}\,G^{--}(\varepsilon,\mathbf{p}),\\ G^{-+}(\varepsilon,\mathbf{p})&=i\,[1-\mathrm{th}(\varepsilon/2T)]\,\mathrm{Im}\,G^{--}(\varepsilon,\mathbf{p}).\end{aligned}\tag{6}$$

We express now the function G in terms of more convenient diagram elements, viz., self-energy functions. The Keldysh technique makes use of four such functions: $\Sigma^{--},\Sigma^{++}m\Sigma^{+-}$, and Σ^{-+}, which satisfy the relation

$$\Sigma^{++}+\Sigma^{--}=-(\Sigma^{+-}+\Sigma^{-+}).$$

The functions Σ^{+-} and Σ^{-+} are pure imaginary, while Σ^{++} and Σ^{--} are related by an equation similar to (5)[2)]:

$$\Sigma^{++}=-(\Sigma^{--})^{*}.\tag{7}$$

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The four G functions are connected with the Σ functions by the matrix equation

$$G_0^{-1}G=\sigma_z+\sigma_z\Sigma G, \quad (8)$$

where

$$G=\begin{pmatrix} G^{--} & G^{-+} \\ G^{+-} & G^{++}\end{pmatrix}, \quad \Sigma=\begin{pmatrix} \Sigma^{--} & \Sigma^{-+} \\ \Sigma^{+-} & \Sigma^{++}\end{pmatrix}, \quad \sigma_z=\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}.$$

In terms of Fourier components, this equation reduces to a set of algebraic equations. Solving this set, we get

$$G^{--}=(G_0^{-1}+\Sigma^{++})/D, \quad G^{-+}=-\Sigma^{-+}/D,$$
$$G^{+-}=-\Sigma^{+-}/D, \quad G^{++}=-(G_0^{-1}-\Sigma^{--})/D, \quad (9)$$

where $G_0^{-1}=\varepsilon-\varepsilon_0(p)$, $\varepsilon_0(p)$ is the "unperturbed" roton energy at $T=0$, and D is a real quantity:

$$D=(G_0^{-1}+\Sigma^{++})(G_0^{-1}-\Sigma^{--})+\Sigma^{+-}\Sigma^{-+}. \quad (10)$$

Using now the connection between the G functions (5) and (6), we see from (9) and (10) that the self-energy functions Σ are connected by a relation similar to (6):

$$\Sigma^{+-}=-i[1+\mathrm{th}\,(\varepsilon/2T)]\ \mathrm{Im}\,\Sigma^{--},$$
$$\Sigma^{-+}=-i[1-th\,(\varepsilon/2T)]\ \mathrm{Im}\,\Sigma^{--}. \quad (11)$$

For rotons we have

$$e^{-\varepsilon/T}\approx e^{-\Delta/T}\ll 1. \quad (12)$$

Neglecting terms of order $\exp(-\varepsilon/T)$ we get ultimately

$$G^{+-}\approx-\Sigma^{+-}[(\varepsilon-\varepsilon_0(p)-\Sigma')^2+{}^1/_4|\Sigma^{+-}|^2]^{-1}, \quad (13)$$

where $\Sigma'(\varepsilon,\mathbf{p})=\mathrm{Re}\,\Sigma^{--}(\varepsilon,\mathbf{p})$.

We are not interested here in the shift of the roton line, but only in its shape. this shape, as seen from (13), is determined by the function $\Sigma^{+-}(\varepsilon,\mathbf{p})$. We shall see that in this energy-shift region we have

$$\omega=\varepsilon-\varepsilon(p)$$

($\varepsilon(\mathbf{p})$ is the roton energy), in which Σ^{+-} is independent of ω, the line shape is Lorentzian of width $\gamma=|\Sigma^{+-}|$. We shall show below that this takes place only for $|\omega|\ll T$. For larger $|\omega|$ the line deviates from Lorentzian.

3. CALCULATION OF $\Sigma^{+-}(\varepsilon,\mathbf{p})$

When Σ^{+-} is calculated in the first nonvanishing perturbation theory approximation, the Keldysh diagram technique uses the two diagrams shown in Fig. 1 [P_i stand for the 4-vectors $(\varepsilon_i,\mathbf{p}_i)$]. The dashed lines describe here the interaction between the rotons; dashed lines with "plus" and "minus" signs correspond respectively to $+iV$ and $-iV$, where V is the Fourier component of the roton-interaction energy. When diagrams of higher order are added to those of Fig. 1, it must be recognized that by virtue of (12) the rotons obey Boltzmann statistics with high accuracy. In the language of Green's functions, this is manifested in the fact that $|G^{-+}|\ll|G^{+-}|$ according to (6). This means that no additional G^{-+} factors appear when dashed lines are added to the diagrams of Fig. 1. In addition, one can choose for the functions G^{--} and G^{++} their values at absolute zero temperature. It turns out as a result that we need sum only "ladder" diagrams of the form shown in Fig. 2. In these diagrams, all the positive dashed lines are in the left-hand part of the diagrams, and the negative in the right one. In fact, addition of a negative dashed line between positive ones would lead to the appearance of extra factors G^{-+}, while diagrams with crossing dashed lines are equal to zero at $T=0$ [Ref. 10, §16]. (See the analogous reasoning in the derivation of the kinetic equation in the Baym-Kadanoff technique.[11]).

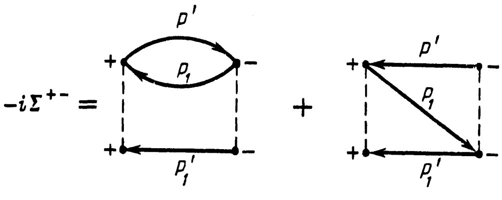

FIG. 1.

It is known that a diagram series of the type shown in Fig. 3 has its sum the quantity $i\Gamma(P',P_1';P,P_1)$ representing the total vertex part of roton-roton scattering. On the "physical" surface, i.e., when the energies of all rotons are equal to $\varepsilon(p)$, this is the roton-roton scattering amplitude. As to the series shown in Fig. 4, its sum is $i\Gamma^{++}(P',P_1';P,P_1)$ and it can be shown that

$$\Gamma^{++}(P',P_1';P,P_1)=-\Gamma^*(P,P_1;P',P_1'). \quad (14)$$

As a result, the sum of diagrams of the type shown in Figs. 2a and 2b, is equal to

$$-i\Sigma^{+-}(P)=\frac{i}{2}\int|\Gamma(P',P_1';P,P_1)|^2G^{-+}(P_1)$$
$$\times G^{+-}(P')G^{+-}(P_1')\frac{d^4P_1\,d^4P'}{(2\pi)^8}, \quad (15)$$

where $P+P_1=P'+P_1'$.

When the condition (12) as well as the natural requirement $\gamma\ll\Delta$ are taken into account, it is necessary to use for G^{+-} and G^{-+} the expressions

$$G^{+-}(\varepsilon,\mathbf{p})=-2\pi i\delta(\varepsilon-\varepsilon(p)),$$
$$G^{-+}(\varepsilon,\mathbf{p})=-2\pi in(\mathbf{p})\delta(\varepsilon-\varepsilon(p)), \quad (16)$$

where $n(\mathbf{p})=\exp[-\varepsilon(p)/T]$ is the Boltzmann distribution function. The use of Eqs. (16) means neglect of the δ-function smearing due to the collisions between the rotons. This smearing is of the order of the linewidth γ. This effect can be neglected if $\gamma\lesssim T$.

Integrating over $d\varepsilon_1$ and $d\varepsilon'$, we reduce (15) to the form

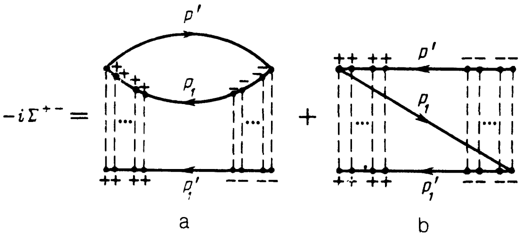

FIG. 2.

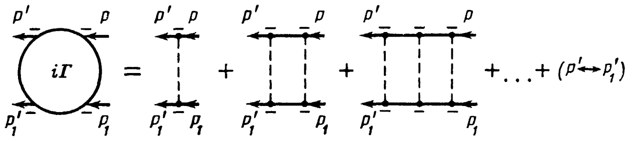

FIG. 3.

$$-i\Sigma^{+-}=2\pi\int w(P',P_1';P,P_1)\delta[\omega+\varepsilon(p)+\varepsilon(p_1)-\varepsilon(p')-\varepsilon(p_1')]n(\mathbf{p}_1)\frac{d^3\mathbf{p}_1\,d^3\mathbf{p}'}{(2\pi)^6}, \quad (17)$$

with $\mathbf{p}+\mathbf{p}_1=\mathbf{p}'+\mathbf{p}_1'$. We have introduced the roton-scattering probability

$$w(P',P_1';P,P_1)={}^1/_2|\Gamma(P',P_1';P,P_1)|^2.$$

It is important in what follows that the major contributions to the integrals over $d^3\mathbf{p}_1$ and $d^3\mathbf{p}'$ is made by values of p_1 and p' that are close to p_0:

$$|p_1-p_0|,\ |p'-p_0|\sim\max\,[(\mu T)^{1/2},\ (\mu\omega)^{1/2}]\ll p_0$$

(μ is the roton effective mass). The momentum p of the created roton will also be assumed close to p_0: $|p-p_0|\ll p_0$. The angles θ_0 between $\mathbf{p}$ and $\mathbf{p}_1$ and θ_1 between $\mathbf{p}'$ and $\mathbf{p}_1'$ are therefore close to the angle defined by the equality

$$2p_0\sin(\theta/2)=|\mathbf{p}+\mathbf{p}_1|.$$

We direct the z axis along the vector of the summary roton momentum $\mathbf{p}+\mathbf{p}_1$, and introduce in place of $\mathbf{p}'$ the variables q, q_2, and φ' defined by

$$p_x'=[p_0\sin(\theta/2)+q]\cos\varphi',\quad p_y'=[p_0\sin(\theta/2)+q]\sin\varphi',\quad p_z'=p_0\cos(\theta/2)+q_z,$$

where $|q|$, $|q_z|\ll p_0$. The dependene of the probability w on q and q_2 can be neglected, and the argument of the δ function in (17) takes the form

$$\omega+[(p-p_0)^2+(p_1-p_0)^2]/2\mu-[q^2\sin^2(\theta/2)+q_z^2\cos^2(\theta/2)]/\mu.$$

Introducing the notation

$$\gamma=-i\Sigma^{+-}$$

and recognizing that w depends only on the angles θ and φ between the planes $(\mathbf{p},\mathbf{p}_1)$ and $(\mathbf{p}',\mathbf{p}_1')$, we reduce (17) to the form

$$\gamma=N_p\frac{p_0\mu}{2}\int\limits_{|x|>x_0}e^{-x^2}\frac{dx}{\pi^{1/2}}\frac{w}{\cos(\theta/2)}\frac{do}{4\pi}, \quad (18)$$

where N_p is the number of rotons per unit volume, $x=(p_1-p_0)(2\mu T)^{-1/2}$, $do=\sin\theta d\theta d\varphi$ is the solid angle of the vector $\mathbf{p}_1$, and

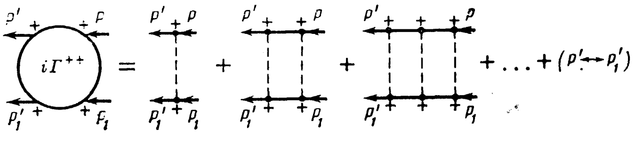

FIG. 4.

$$x_0=\begin{cases}0, & \omega+(p-p_0)^2/2\mu\geq 0\\ |\omega|/T-(p-p_0)^2/2\mu T, & \omega+(p-p_0)^2/2\mu<0\end{cases}.$$

The integration in (18), as already mentioned, is in fact over values of p_1 close to p_0, i.e.,

$$|x|\sim(1,\ (|\omega|/T)^{1/2}).$$

Investigation of the diagrams of Fig. 3 shows that the vertex part Γ (hence the probability w) is in this region a slowly varying logarithmic function of the summary roton energy[12,13]:

$$E=\varepsilon(p)+\varepsilon(p_1)+\omega.$$

Neglecting this dependence, we can take w outside the integral over dx.[3)] The result is a final equation for γ (in the usual units)

$$\gamma=\gamma_0\begin{cases}1, & \omega+(p-p_0)^2/2\mu\geq 0\\ 1-\Phi([|\omega|/T-(p-p_0)^2/2\mu T]^{1/2}), & \omega+(p-p_0)^2/2\mu<0\end{cases}, \quad (19)$$

where $\gamma_0=N_p\,p_0\,\mu\overline{w}/2\hbar^3$, Φ is the probability integral, and

$$\overline{w}=\int\frac{w}{\cos(\theta/2)}\frac{do}{4\pi},$$

with the value of w taken for $E-2\Delta\sim T$.

We note now that $\overline{w}$ is precisely the same scattering probability that determines, according to Fomin,[13] the viscosity η and the thermal conductivity $\varkappa$ of helium in the roton region. Thus, for example, the viscosity is $\eta=2p_0\hbar^4/15\mu^2\overline{w}$. It follows from the experimental data on the viscosity that $w=25.2\cdot10^{-76}$ erg$^2\cdot$cm^6, so that $\gamma_0[\mathrm{K}]=47\,T^{1/2}\exp[-\Delta(T)/T]$.

The connection we obtained between the roton viscosity and the roton linewidth has already been used to interpret experimental data (see, e.g., Ref. 1). It was derived previously, however, by applying the Born approximation to roton sattering, assuming a δ-function interaction between the rotons, which certainly does not take place. We see now that this connection is quite general and is valid for any roton-scattering law. The fact that the viscosity, thermal conductivity, and linewidth are determined by one and the same scattering probability $\overline{w}$ can be easily understood by noting that the quantity $-n(p)i\Sigma^{+-}$ is none other than the "departure" term in the collision integral of the kinetic equation. The viscosity and thermal conductivity are usually determined not only by the "departure" but also by the "arrival" terms. A peculiarity of the rotons, on the other hand, according to Ref. 13, that the correction to the equilibrium distribution function is an odd function of $p-p_0$ at $p\approx p_0$. This causes the "arrival" terms, in which the distribution function is integrated over $d^3\mathbf{p}$ to be small in the parameter $(\mu T)^{1/2}/p_0$, so that in fact η and $\varkappa$ are also determined only by the "departure."

4. LINE SHAPE

It follows from the foregoing that the roton-creation line shape is given by

$$S(\varepsilon,\mathbf{p})\propto\gamma/(\omega^2+\gamma^2/4), \quad (20)$$

with γ determined by Eq. (19). It is seen from this formula

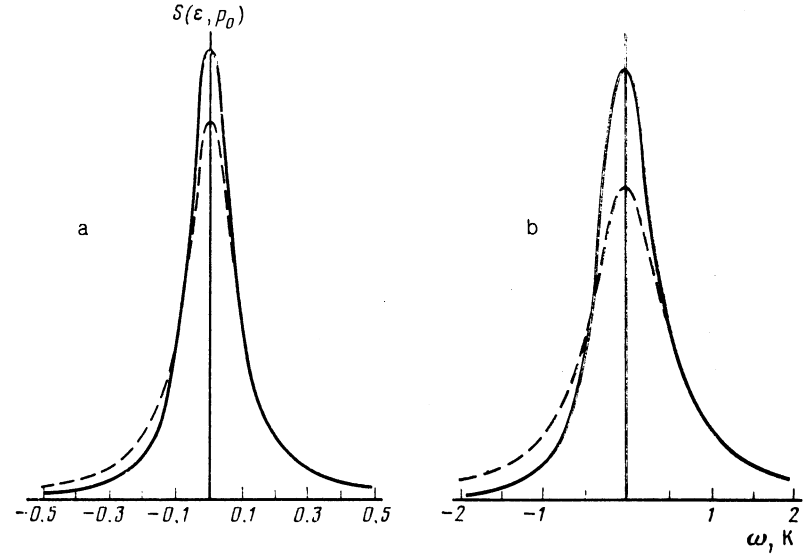

FIG. 5. Probability of roton production by a slow neutron at $p = p_0$ versus the difference ω between the energy transfer ε and the roton energy $\varepsilon(p)$: a — $T_1 = 1.5$ K b — $T_2 = 2$ K.

that $\gamma = \gamma_0$ for all positive ω (i.e., for $\varepsilon \gg \varepsilon(p)$), and that on this wing the line is a Lorentzian of constant width γ_0. For negative ω, however, the situation is different: $\gamma_0 = \gamma_0$ only in the region $|\omega + (p-p_0)^2/2\mu| \ll T$. In the opposite limiting case the scattering intensity decreases more rapidly. We note also that Eq. (19) for γ has a singularity $\omega + (p-p_0)^2/2\mu = 0$. This singularity is due to replacement of the Green's functions in (15) by δ functions, and has no physical meaning. To determine the line shape more precisely in this region, it is necessary to smear out the δ functions with account taken of the fact that γ is finite. With this procedure implemented, Fig. 5 shows the line shape for $p = p_0$ and for two temperatures, $T_1 = 1.5$ K and $T_2 = 2$ K. The corresponding values of γ_0 are respectively 0.17 and 1.06 K. The dashed curves in the figures correspond to a lorentz line symmetric about ω. We see that the line shape deviates substantially from logarithmic at $\omega < -\gamma_0/2$.

The available experimental data[14] indicate apparently that the "negative" wing of the roton line ($\omega < 0$), at least for large $|\omega|$, is noticeably lower than the positive one. A quantitative comparison with theory, on the other hand, calls for investigations at higher resolution. Such measurements can probably be made only by Mezei's neutron spin echo method.[1]

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[1)]For example, the probability of conversion of two rotons into two phonons is low by virtue of the smallness of the phase space of the phonons, i.e., by virtue of the smallness of the parameter Δ/cp_0.

[2)]The authors of Ref. 3 used retarded and advanced Green's functions and a corresponding vertex part $\Sigma_{11} = \sigma^{--} + \Sigma^{-+}$. They used, however, the relation $\Sigma_{11}(-\varepsilon) = \Sigma_{11}^*(\varepsilon)$, which in our opinion does not hold in general. The proof of this relation in Ref. 8 is not convincing. Reference 9, on the other hand, contains the relation $\mathscr{G}(-\omega_\nu) = \mathscr{G}^*(\omega_\nu)$ for Matsubara functions of discrete frequencies. This relation, however, can be shown to be the equivalent of (7) and contradicts the relation used in Ref. 3.

[3)]A more detailed investigation shows that this approximation is accurate to $\approx 15\%$ for $|\omega| \sim T$. Note also that for $|\omega| \ll T$ the linewidth γ is expressed exactly in terms of the quantity $\overline{w}$ introduced in Ref. 13, without neglect of the $w(E)$ dependence.

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